Improved Non-Pt Alloys for the Oxygen Reduction Reaction at Fuel Cell Cathodes Predicted from Quantum Mechanics

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Table S1. Lattice parameter of Y_3X cubic cell, where Y is the noble metal and X is the base metal.

Base\Noble (Angstrom)	Pd	Pt	Rh
Ag	3.989	4.012	3.923
Au	3.998	4.022	3.929
Cd	4.022	4.047	3.955
Co	3.875	3.899	3.794
Cr	3.915	3.927	3.807
Cu	3.881	3.907	3.804
Fe	3.898	3.925	3.812
Hg	4.044	4.073	3.979
Ir	3.923	3.953	3.849
Mn	3.930	3.940	3.817
Mo	3.953	3.982	3.868
Nb	3.979	4.008	3.901
Ni	3.868	3.889	3.789
Os	3.909	3.944	3.841
Pd	3.944	3.968	3.868
Pt	3.953	3.979	3.876
Re	3.936	3.955	3.850
Rh	3.922	3.947	3.841
Ru	3.915	3.940	3.836
Sc	4.003	4.013	3.935
Ta	3.967	4.001	3.894
Tc	3.949	3.950	3.848
Ti	3.927	3.957	3.857
V	3.904	3.929	3.811
W	3.947	3.982	3.811
Y	4.124	4.133	3.867
Zn	3.916	3.939	3.836
Zr	4.024	4.055	3.966

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Table S2. Segregation energy of alloys of 4, 5, and 6 layer slabs.

Alloy\Layers Segregation Energy (eV)	4 Layers	5 Layers	6 Layers
Pt_3Ti	-0.82	-0.91	-0.89
Pt_3Fe	0.10	0.12	0.11
Pt_3Co	0.50	0.40	0.39
Pt_3Ni	0.46	0.37	0.38

Table S3. Optimized spin in e^- of [4 layer uniform slabs / bulk cubic cells].

Base\Noble (spin in e^-) (slab / bulk)	Pd	Pt	Rh
Ag	0.1 / 0	0 / 0	3.7 / 0.5
Au	0.2 / 0	0 / 0	4.8 / 1.5
Cd	0 / 0	0 / 0	0 / 0
Co	13.0 / 3.1	12.6 / 3.1	13.4 / 3.3
Cr	13.4 / 3.0	11.7 / 2.7	8.8 / 1.4
Cu	0 / 0	0 / 0	3.3 / 0
Fe	17.2 / 4.3	17.6 / 4.5	17.2 / 3.8
Hg	0 / 0	0 / 0	0.4 / 0
Ir	0 / 0	0 / 0	0 / 0
Mn	18.7 / 4.7	17.6 / 4.3	14.1 / 2.6
Mo	4.9 / 2.1	2.1 / 1.9	0 / 0
Nb	0 / 1.0	0 / 0.6	0 / 0
Ni	6.0 / 1.8	6.3 / 1.2	9.1 / 2.3
Os	0.1 / 0.0	0.1 / 0	0.3 / 0
Pd	4.7 / 0	0.1 / 0.2	6.3 / 0.3
Pt	0.7 / 0.4	2.8 / 0	3.1 / 0
Re	7.2 / 2.3	5.1 / 0	0 / 0
Rh	4.2 / 0	0.6 / 0.1	0.2 / 0
Ru	10.1 / 0.5	1.2 / 0	0.4 / 0
Sc	0 / 0	0 / 0	0 / 0
Ta	0 / 0.7	0 / 0.1	0 / 0
Tc	11.1 / 3.0	6.5 /	0 / 0
Ti	0 / 0	0 / 0	0 / 0
V	3.0 / 1.3	1.3 / 1.3	0.8 / 0
W	3.1 / 2.0	2.9 / 1.7	0 / 0
Y	0 / 0	0 / 0	0 / 0
Zn	0 / 0	0 / 0	0 / 0
Zr	0 / 0	0 / 0	0 / 0